

CONVERGENCE OF A FORCE-BASED HYBRID METHOD FOR ATOMISTIC AND CONTINUUM MODELS IN THREE DIMENSION

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ABSTRACT. We study a force-based hybrid method that couples atomistic models with nonlinear Cauchy-Born elasticity models. We show that the proposed scheme converges quadratically to the solution of the atomistic model, as the ratio between lattice parameter and the characteristic length scale of the deformation tends to zero. Convergence is established for general short-ranged atomistic potential and for simple lattices in three dimension. The convergence is based on consistency and stability analysis. General tools are developed in the framework of pseudo-difference operators for stability analysis in arbitrary dimension of the multiscale atomistic and continuum coupling methods.

1. INTRODUCTION

Multiscale methods for mechanical deformation of materials have been investigated intensely in recent years. The main spirit of these methods is to use atomistic models for regions containing defects, and continuum models in regions where the material is smoothly deformed. We refer to the recent review [29] for various methods and the book [20] for general discussion of multiscale modeling.

There are two different ways of coupling atomistic and continuum models. One is based on energy, and the other is based on force. The energy-based method defines an energy which is a mixture of atomistic energy and continuum elasticity energy. The energy functional is then minimized to obtain the solution. The force-based method works instead at the level of force balance equations. The forces derived from atomistic and continuum models are coupled together. The force balance equations are solved to obtain the deformed state of the system.

From a numerical analysis point of view, one of the key issues for these multiscale methods is the consistency and stability of the coupled schemes. Taking one of the most successful multiscale methods, the quasicontinuum method [26, 38] for

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example, one of the main issues is the so called ghost force problem [35], which are the artificial non-zero forces that the atoms experience at their equilibrium state. In the language of numerical analysis, it means that the scheme lacks consistency at the interface between atomistic and continuum regions [16]. In [30], it was shown that the ghost forces may lead to a finite size error of the gradient of the solution.

The stability analysis for the coupling schemes is so far limited to one dimensional systems, in which case a direct calculation is possible thanks to the easy one dimensional lattice structure and pairwise interaction potential. This is no longer the case in two and three dimensions, and the extension is by no means easy. More general tools for stability analysis are needed, to address in general the multiscale hybrid methods.

In this work, based on existing ideas in the literature, we formulate a force-based hybrid scheme for general short-ranged potentials (with some natural assumptions) in three dimension. We focus on the numerical analysis of the hybrid method, which is a representative of a general class of multiscale methods. The solution of the proposed method converges quadratically to the solution of the atomistic model as the ratio between lattice parameter and the characteristic length scale of the mechanical deformation goes to zero. To the best of our knowledge, this is the first convergence result for multiscale methods coupling atomistic and continuum models in three dimension.

The convergence result is based on the analysis of consistency and linear stability. To achieve this, we study the linearized operator in the framework of pseudo-difference operators. We obtained the stability estimate combining regularity estimate of pseudo-difference operators, consistency of the linearized operator, and stability of the continuous problem. These tools developed will help understanding multiscale methods in general.

Before we present the formulation of the method and the main theorem in Section 1.3, we need some preliminaries and notations.

1.1. Lattice function and norms. We will consider only Bravais lattices (see for example [3]) in this work, denoted as \mathbb{L} . Let d be the dimension. Let $\{a_j\} \subset \mathbb{R}^d$, $j = 1, \dots, d$ be basis vectors of the lattice \mathbb{L} , hence

$$\mathbb{L} = \{x \in \mathbb{R}^d \mid x = \sum_j n_j a_j, n \in \mathbb{Z}^d\}.$$

Let $\{b_j\} \subset \mathbb{R}^d$, $j = 1, \dots, d$ be the reciprocal basis vectors, given by

$$a_j \cdot b_k = 2\pi \delta_{jk}.$$

The reciprocal lattice \mathbb{L}^* is then

$$\mathbb{L}^* = \{x \in \mathbb{R}^d \mid x = \sum_j n_j b_j, n \in \mathbb{Z}^d\}.$$

Denote the unit cells of \mathbb{L} and \mathbb{L}^* as Γ and Γ^* respectively.

$$\Gamma = \{x \in \mathbb{R}^d \mid x = \sum_j c_j a_j, 0 \leq c_j < 1, j = 1, \dots, d\};$$

$$\Gamma^* = \{x \in \mathbb{R}^d \mid x = \sum_j c_j b_j, -1/2 \leq c_j < 1/2, j = 1, \dots, d\}.$$

For $\varepsilon = 1/n$, $n \in \mathbb{Z}_+$, we will consider lattice system $\varepsilon\mathbb{L}$ inside domain $\Omega = \Gamma \subset \mathbb{R}^d$, denoted as $\Omega_\varepsilon = \Omega \cap \varepsilon\mathbb{L}$. Note that the lattice constant is ε , so that the number of points in Ω_ε is $1/\varepsilon^d$. We will restrict to periodic boundary conditions in this work, general boundary conditions will be leaved for future publications. For a lattice function u defined on $\varepsilon\mathbb{L}$, we say it is Ω_ε -periodic if

$$u(x) = u(x'), \quad \forall x, x' \in \varepsilon\mathbb{L}, x - x' = a_j \text{ for some } j \in \{1, \dots, d\}.$$

In particular, an Ω_ε -periodic function is determined by its restriction on Ω_ε . Functions defined on Ω_ε can be easily extended to Ω_ε -periodic functions defined on $\varepsilon\mathbb{L}$.

We also define the reciprocal lattice associated with Ω_ε . Let $\mathbb{L}_\varepsilon^* = \mathbb{L}^* \cap (\Gamma^*/\varepsilon)$. Define K_ε a subset of \mathbb{Z}^d given by

$$K_\varepsilon = \{\mu \in \mathbb{Z}^d \mid \sum_j \varepsilon \mu_j b_j \in \Gamma^*\},$$

hence \mathbb{L}_ε^* is given by

$$\mathbb{L}_\varepsilon^* = \{x \in \mathbb{R}^d \mid x = \sum_j \mu_j b_j, \mu \in K_\varepsilon\}.$$

For $\mu \in \mathbb{Z}^d$, the translation operator T_ε^μ is defined as

$$(T_\varepsilon^\mu u)(x) = u(x + \varepsilon \mu_j a_j), \quad \text{for } x \in \mathbb{R}^d.$$

We define the forward and backward discrete gradient operators as

$$D_{\varepsilon,s}^+ = \varepsilon^{-1}(T_\varepsilon^\mu - I) \quad \text{and} \quad D_{\varepsilon,s}^- = \varepsilon^{-1}(I - T_\varepsilon^\mu),$$

where $s = \sum_i \mu_i a_i$ and I denotes the identity operator. It is easy to see $D_{\varepsilon,-s}^+ = -D_{\varepsilon,s}^-$.

We say α is a multi-index, if $\alpha \in \mathbb{Z}^d$ and $\alpha \geq 0$. We will use the notation

$$|\alpha| = \sum_{j=1}^d \alpha_j.$$

For a multi-index α , the difference operator D_ε^α is given by

$$D_\varepsilon^\alpha = \prod_{j=1}^d (D_{\varepsilon,a_j}^+)^{\alpha_j}.$$

When no confusion will occur, we will omit the subscript ε in the notations T_ε^μ , $D_{\varepsilon,s}^+$, $D_{\varepsilon,s}^-$ and D_ε^α for simplicity.

We will use various norms for functions defined on the lattice Ω_ε . For integer $k \geq 0$, define the difference norm

$$\|u\|_{\varepsilon,k}^2 = \sum_{0 \leq |\alpha| \leq k} \varepsilon^d \sum_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|^2.$$

It is clear that $\|\cdot\|_{\varepsilon,k}$ is a discrete analog of Sobolev norm associated with $H^k(\Omega)$. Hence, we denote the corresponding spaces of lattice functions as $H_\varepsilon^k(\Omega)$ and $L_\varepsilon^2(\Omega)$ when $k = 0$. We also need the uniform norms on the lattice Ω_ε , given by

$$\begin{aligned} \|u\|_{L_\varepsilon^\infty} &= \max_{x \in \Omega_\varepsilon} |u(x)|, \\ \|u\|_{W_\varepsilon^{k,\infty}} &= \sum_{0 \leq |\alpha| \leq k} \max_{x \in \Omega_\varepsilon} |(D_\varepsilon^\alpha u)(x)|. \end{aligned}$$

In the above definitions, we have identified lattice function u with its Ω_ε -periodic extension to function defined on $\varepsilon\mathbb{L}$, and hence the differences are well-defined. These norms extend to vector-valued functions as usual.

Define the discrete Fourier transform for lattice functions f as

$$(1.1) \quad \widehat{f}(\xi) = \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-ix \cdot \xi} f(x), \quad \xi \in \mathbb{L}_\varepsilon^*,$$

and its inverse as

$$(1.2) \quad f(x) = (2\pi)^{d/2} \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \widehat{f}(\xi), \quad x \in \Omega_\varepsilon.$$

We need a symbol which plays the same role for difference operators that $\Lambda^2(\xi) = 1 + \Lambda_0^2(\xi) = 1 + |\xi|^2$ plays for differential operators. For $\varepsilon > 0$, $\xi \in \mathbb{L}_\varepsilon^*$, let

$$\Lambda_{j,\varepsilon}(\xi) = \frac{1}{\varepsilon} |e^{i\varepsilon\xi_j} - 1|, \quad j = 1, \dots, d,$$

and

$$\Lambda_\varepsilon^2(\xi) = 1 + \Lambda_{0,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \Lambda_{j,\varepsilon}^2(\xi) = 1 + \sum_{j=1}^d \frac{4}{\varepsilon^2} \sin^2\left(\frac{\varepsilon\xi_j}{2}\right).$$

It is not hard to check for any $\xi \in \mathbb{L}_\varepsilon^*$, it holds

$$(1.3) \quad c\Lambda^2(\xi) \leq \Lambda_\varepsilon^2(\xi) \leq \Lambda^2(\xi).$$

where the positive constant c depends on $\{b_j\}$.

The L_ε^2 norm of lattice function can be rewritten as

$$(1.4) \quad \|f\|_{\varepsilon,0}^2 = (2\pi)^d \sum_{\xi \in \mathbb{L}_\varepsilon^*} |\widehat{f}(\xi)|^2.$$

Indeed, using Poisson summation formula,

$$\begin{aligned}
\sum_{\xi \in \mathbb{L}_\varepsilon^*} |\widehat{f}(\xi)|^2 &= \sum_{\xi \in \mathbb{L}_\varepsilon^*} \varepsilon^{2d} (2\pi)^{-d} \sum_{x \in \Omega_\varepsilon} e^{i\xi \cdot x} f^*(x) \sum_{x' \in \Omega_\varepsilon} e^{-i\xi \cdot x'} f(x') \\
&= \sum_{x, x' \in \Omega_\varepsilon} \varepsilon^{2d} (2\pi)^{-d} f^*(x) f(x') \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{i\xi \cdot (x-x')} \\
&= \sum_{x \in \Omega_\varepsilon} (2\pi)^{-d} \varepsilon^d |f(x)|^2 = (2\pi)^{-d} \|f\|_{\varepsilon,0}^2.
\end{aligned}$$

Moreover, notice that for $\xi \in \mathbb{L}_\varepsilon^*$, we have

$$\widehat{D_{\varepsilon, a_j}^+ f}(\xi) = \frac{1}{\varepsilon} (e^{i\varepsilon \xi \cdot a_j} - 1) \widehat{f}(\xi).$$

Therefore, discrete Sobolev norms have equivalent representations using discrete Fourier transform:

$$c \|f\|_{\varepsilon, k}^2 \leq \sum_{\xi \in \mathbb{L}_\varepsilon^*} \Lambda_\varepsilon^k(\xi) |\widehat{f}(\xi)|^2 \leq C \|f\|_{\varepsilon, k}^2,$$

with positive constant c depending on k and $\{a_j\}$.

For $k > d/2$, we have the following discrete Sobolev imbedding inequality [24, Proposition 6]:

$$\|f\|_{L_\varepsilon^\infty} \leq C \|f\|_{\varepsilon, k},$$

where C depends on k and Ω .

1.2. Atomistic model and Cauchy-Born rule. In this work, we will restrict our attention to classical empirical potentials. For atoms located at $\{y_1, \dots, y_N\}$, the interaction potential energy between the atoms is given by

$$V(y_1, \dots, y_N),$$

where V often takes the form:

$$V(y_1, \dots, y_N) = \sum_{i,j} V_2(y_i/\varepsilon, y_j/\varepsilon) + \sum_{i,j,k} V_3(y_i/\varepsilon, y_j/\varepsilon, y_k/\varepsilon) + \dots$$

Here we have omitted interactions of more than three atoms.

Different potentials are chosen for different materials. In this paper, we will work with general atomistic models, and we will make the following assumptions on the potential functions V as in [19]:

- (1) V is translation invariant.
- (2) V is invariant with respect to rigid body motion.
- (3) V is smooth in a neighborhood of the equilibrium state.
- (4) V has finite range and consequently we will consider only interactions that involve a finite number of atoms.

The first two assumptions are general [8], while the latter two are specific technical assumptions.

In fact, for simplicity of notation and clarity of presentation, our presentation will be limited to potentials that contain only two-body and three-body potentials. Actually, we will sometimes only make explicit the three-body terms in the expressions for the potential and omit the two-body terms. It is straightforward to extend our results to potentials with interactions of more atoms that satisfy the above conditions, following the discussion on the three-body terms. By [25], the potential function V is a function of atom distances and angles by invariance with respect to rigid body motion. Therefore, we may write

$$\begin{aligned} V_2(y_i, y_j) &= V_2(|y_i - y_j|^2), \\ V_3(y_i, y_j, y_k) &= V_3(|y_i - y_j|^2, |y_i - y_k|^2, \langle y_i - y_j, y_i - y_k \rangle), \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product over \mathbb{R}^d . We write the two-body and three-body potentials this way to make the formula in our calculations easier to read.

We assume that the atoms are located at Ω_ε in equilibrium, with x denoting the equilibrium position ($x \in \Omega_\varepsilon$). Positions of the atoms under deformation will be viewed as a function defined over Ω_ε , denote as $y(x) = x + u(x)$. Hence, $u : \Omega_\varepsilon \rightarrow \mathbb{R}^d$ is the displacement of atoms. We extend u as an Ω_ε -periodic function defined on $\varepsilon\mathbb{L}$. Denote the space of atom positions y as

$$X_\varepsilon = \{y : \varepsilon\mathbb{L} \rightarrow \mathbb{R}^d \mid y = x + u, u \text{ } \Omega_\varepsilon\text{-periodic}, \sum_{x \in \Omega_\varepsilon} u(x) = 0\}.$$

Hence, $y \in X_\varepsilon$ satisfies

$$y(x) - y(x') = x - x', \quad \forall x, x' \in \varepsilon\mathbb{L}, x - x' = a_j \text{ for some } j \in \{1, \dots, d\}.$$

The atomistic problem is formulated as follows. For given $f : \Omega_\varepsilon \rightarrow \mathbb{R}^d$, find $y \in X_\varepsilon$ such that

$$(1.5) \quad y = \arg \min_{z \in X_\varepsilon} I_{\text{at}}(z),$$

where

$$I_{\text{at}}(z) = \frac{1}{3!} \varepsilon^d \sum_{x \in \Omega_\varepsilon} \sum_{(s_1, s_2) \in S} V_{(s_1, s_2)}[z] - \varepsilon^d \sum_{x \in \Omega_\varepsilon} f(x)z(x),$$

where

$$V_{(s_1, s_2)}[z] = V(|D_{s_1}^+ z(x)|^2, |D_{s_2}^+ z(x)|^2, \langle D_{s_1}^+ z(x), D_{s_2}^+ z(x) \rangle).$$

Here S is the set of all possible (s_1, s_2) within the range of the potential. By our assumptions, S is a finite set. Note that as remarked above, we only make explicit the three body terms in the potential. In I_{at} , ε^d is a normalization factor, so that I_{at} is actually the energy of the system per atom.

The Euler-Lagrange equations for the atomistic problem is then

$$(1.6) \quad \mathcal{F}_{\text{at}}[y](x) = f(x), \quad x \in \Omega_\varepsilon,$$

where

$$\begin{aligned} \mathcal{F}_{\text{at}}[y](x) = & \sum_{(s_1, s_2) \in S} \left(D_{s_1}^- \left(2\partial_1 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x) \right) \right. \\ & \left. + D_{s_2}^- \left(2\partial_2 V_{(s_1, s_2)}[y](x) D_{s_2}^+ y(x) + \partial_3 V_{(s_1, s_2)}[y](x) D_{s_1}^+ y(x) \right) \right), \end{aligned}$$

where for $i = 1, 2, 3$, we denote

$$\partial_i V_{(s_1, s_2)}[y](x) = \partial_i V \left(|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle \right),$$

the partial derivative with respect to the i -th argument of V .

To introduce the continuum Cauchy-Born (CB) elasticity problem [8, 21, 22], we fix more notations. For any positive integer k , we denote by $W^{k,p}(\Omega; \mathbb{R}^d)$ the Sobolev space of mappings $y: \Omega \rightarrow \mathbb{R}^d$ such that $\|y\|_{W^{k,p}} < \infty$. In particular, $W_{\#}^{k,p}(\Omega; \mathbb{R}^d)$ denotes the Sobolev space of periodic functions whose distributional derivatives of order less than k are in the space $L^p(\Omega)$. For any $p > d$ and $m \geq 0$, we define X as

$$X = \{y: \Omega \rightarrow \mathbb{R}^d \mid y = x + v, v \in W^{m+2,p}(\Omega; \mathbb{R}^d) \cap W_{\#}^{1,p}(\Omega; \mathbb{R}^d), \int_{\Omega} v = 0\}.$$

As in [19], we have the Cauchy-Born elasticity problem as: find $y \in X$ such that

$$(1.7) \quad y = \arg \min_{z \in X} I(z),$$

where the total energy functional I is given by

$$I(z) = \int_{\Omega} (W_{\text{CB}}(\nabla v(x)) - f(x)z(x)) \, dx,$$

where $v(x) = z(x) - x$ and Cauchy-Born stored energy density W_{CB} is given by

$$W_{\text{CB}}(A) = \frac{1}{3!} \sum_{(s_1, s_2) \in S} W_{(s_1, s_2)}(A),$$

where for $A \in \mathbb{R}^{d \times d}$,

$$W_{(s_1, s_2)}(A) = V \left(|s_1 + s_1 A|^2, |s_2 + s_2 A|^2, \langle s_1 + s_1 A, s_2 + s_2 A \rangle \right).$$

The range S is the same as that in the atomistic potential. We have used the deformed position y instead of the more usual displacement field u as variable in (1.7) in order to be parallel with the atomistic problem.

The Euler-Lagrange equation for the Cauchy-Born elasticity model is then

$$(1.8) \quad \mathcal{F}_{\text{CB}}[y](x) = f(x),$$

where

$$\mathcal{F}_{\text{CB}}[y](x) = -\nabla \cdot (D_A W_{\text{CB}}(\nabla v(x))), \quad v(x) = y(x) - x.$$

Here $D_A W_{\text{CB}}(A)$ denotes differentiation of $W_{\text{CB}}(A)$ with respect to A .

Since we are primarily interested in the coupling between the atomistic and continuum region, we will take the finite element discretization $\mathcal{T}_{\varepsilon}$ be a triangulation of

Ω_ε with each atom site as an element vertex with element size ε . The triangulation is chosen so that it is translation invariant. The approximation space \tilde{X}_ε is defined as

$$\tilde{X}_\varepsilon = \{y \in W_\sharp^{1,p}(\Omega; \mathbb{R}^d) \mid y|_T \in P_1(T), \forall T \in \mathcal{T}_\varepsilon\},$$

where $P_1(T)$ is the space of linear functions on the element T .

1.3. Force-based hybrid method. We are ready to formulate the force-based hybrid method.

We take $\varrho : \Omega \rightarrow [0, 1]$ as a smooth standard cutoff function. The atomistic region corresponds to the zero level set of ϱ : $\Omega_a = \{x \mid \varrho(x) = 0\}$, and the continuum region corresponds to the region that ϱ equals to 1: $\Omega_c = \{x \mid \varrho(x) = 1\}$. The region in between is a buffer between the atomistic and continuum regions.

The force-based hybrid method is given as: find $y(x) \in X_\varepsilon$ such that

$$(1.9) \quad \mathcal{F}_{\text{hy}}[y](x) \equiv (1 - \varrho(x))\mathcal{F}_{\text{at}}[y](x) + \varrho(x)\mathcal{F}_\varepsilon[y](x) = f(x), \quad x \in \Omega_\varepsilon,$$

where \mathcal{F}_ε is the force from finite element approximation of Cauchy-Born elasticity problem (1.7). Due to the choice of ϱ , in the atomistic region Ω_a , the force acting on the atom is just that of atomistic model, while in the continuum region Ω_c , the force is calculated from finite element approximation of the Cauchy-Born elasticity.

The proposed scheme works in dimension $d \leq 3$ for general short-range interaction potentials. The main result for this work is the following quadratic convergence result for the force-based hybrid method.

Theorem 1 (Convergence). *Under Assumptions A and B, there exist positive constants δ and M , so that for any $p > d$ and $f \in W^{15,p}(\Omega) \cap W_\sharp^{1,p}(\Omega)$ with $\|f\|_{W^{15,p}} \leq \delta$, we have*

$$(1.10) \quad \|y_{\text{hy}} - y_{\text{at}}\|_{\varepsilon,2} \leq M\varepsilon^2.$$

Remark. While we do not attempt in this work to optimize the regularity assumption on f , we note that it is easy to relax the assumption to $f \in W^{5,p}(\Omega)$ with $p > d$ following the remarks below in the proof.

Remark. The sharp stability conditions Assumptions A and B will be given in Section 3. These assumptions are quite natural and physical. We refer to Section 3 and also [19] for more discussions on the stability conditions and its link to physics literature.

The proof of Theorem 1, which will be viewed as a convergence result for (non-linear) finite difference schemes, follows the spirit of Strang's work [37]. In short, consistency and linear stability implies convergence. The heart of the matter lies in the analysis of consistency and stability, which will be the focus of the proof.

The rest of the paper is organized as follows. In the next subsection, we review some related works. Section 2 discusses the consistency of the scheme. The linear

stability is proved in Section 4. The stability estimate is based on the regularity estimate of finite difference schemes in Section 3, which is established in the framework of pseudo-difference operators [9, 27, 40]. With the preparation of consistency and linear stability analysis, the proof is concluded in Section 5.

1.4. Related works. Recently there are a lot of papers discussing various atomistic/continuum coupling strategies as summarized in the recent reviews [10, 15, 29, 33], we will only mention some of the works that are closely related to ours and refer the readers to these reviews and the references therein.

The hybrid method resembles several methods in the literature. The most closely related method is the quasicontinuum (QC) method [26, 38], which is among the most popular methods for modeling the mechanical deformation of crystalline solids. The QC method contains following ingredients: decomposition of the whole domain into atomistic and continuum regions, with the defects covered by the atomistic regions; degree reduction by adaptive selection of representative atoms (rep-atoms), with fewer atoms selected in regions with smooth deformation; and the application of the Cauchy-Born approximation in the continuum region to reduce the complexity involved in computing the total energy of the system.

Both the proposed method and QC method couple atomistic models with non-linear Cauchy-Born elasticity model. In some sense, the proposed method can be viewed as a smoothened modification of the force-based QC method. Indeed, the original force-based QC method amounts to take ϱ to be a characteristic function (so that there is no buffer region). The force-based QC is free of ghost force, and it was proven in [12, 31] that, for one-dimensional problem, the force-based method converges quadratically. However, its convergence behavior remains open for high dimensional problem. As will be proved later in the paper, the proposed method is stable and also converges quadratically in three dimension. For the understanding of the original force-based QC, this work may also provide some new tools and insights.

The Arlequin method [5, 7] and the bridging domain method [6] also adopt a smooth transition between atomistic and continuum regions. The difference with the proposed scheme is however these methods are energy-based, so that the mixing is done at the energy level, while the current method is force-based. Moreover, these two methods enforce the consistency between the atomistic and continuum regions by imposing certain constraints, while there is no such constraints in our method. These methods are suffered from ghost force problems as shown in [29], while the proposed method is consistent at the interface.

The proposed method also shares certain common traits with the concurrent AtC coupling method (AtC) proposed in [4]. The AtC method also uses a smooth transition between atomistic and continuum regions and is force-based. However, the proposed method differs from AtC in the following aspects: (1) our method

employs Cauchy-Born elasticity while AtC uses linear elasticity and (2) our method is free of ghost force while AtC is plagued by ghost force as demonstrated in [29].

Most of the analysis of these multiscale methods limits to the quasicontinuum method. In [19], the Cauchy-Born rule for crystalline solids is verified under sharp stability conditions. In the language of QC, the authors in [19] actually proved the convergence of local QC (the whole computational domain is treated as local region). Explicit convergence rate for the local QC can be found in [17, 18].

For the QC method couples together atomistic and continuum models (nonlocal QC method in short), the error estimate can be found in [13, 30] and the references therein. All these works dealt only with the one dimensional problem, and moreover, except [30], the analysis was limited to quadratic potential models, so that the system is linear.

To the best of the authors' knowledge, there is no analysis for the nonlocal QC method or other coupling schemes for high-dimensional problems with general potential (usually, many-body potential function). The main difficulties lie in the analysis of the consistency and stability. For one-dimensional problem, the lattice structure is very simple and the pairwise potential function can be handled by a direct calculation. However, such an approach cannot be easily extended to high-dimensional problem with general potential because the lattice structure and the potential function for high-dimensional problem is much more involved. One of the main contributions of the current paper is the development of general tools for the analysis of consistency and stability.

Finally, we remark that in this work the analysis of the proposed method, especially the stability analysis, is based on analysis of finite difference schemes. The readers might wonder why the analysis is *not* done in the framework of finite element method, as after all, we are dealing with static problems, the systems to be solved are "elliptic"; and moreover, the continuum region is discretized by finite element method. The reason actually lies in the atomistic part, since the force balance equations derived from energy of discrete lattice systems are intrinsically of finite difference type. To the best of our knowledge, there has not been yet a successful way to put the atomistic equations into the framework of finite element analysis. Therefore, to be consistent, we view the finite element approximation in the continuum region also as a finite difference approximation. The proof hence relies on the analysis of finite difference schemes. This may give a reminiscence of the early history about finite element analysis, during when the finite element method was also analyzed in the framework of finite difference schemes [36]. Since the theory of adaptive mesh is well-established for finite element method, it is an interesting question whether one can adopt the finite element analysis framework to analyze these multiscale coupling methods.

2. CONSISTENCY

We study the consistency of the force-based hybrid method in this section. The key is the following lemma, which is a refined version of [19, Lemma 5.1].

Lemma 2.1 (Consistency of Cauchy-Born rule). *For any $y = x + u(x)$ with u smooth, we have*

$$(2.1) \quad \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L^\infty_\varepsilon} \leq C\varepsilon^2 \|u\|_{W^{16,\infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Remark. The consistency estimate is presented in the form of (2.1) for later use in the proof of Proposition 4.2. A bound involves less order of derivatives of u is possible, in fact, it is not hard to see from the proof that we have

$$(2.2) \quad \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L^\infty_\varepsilon} \leq C\varepsilon^2,$$

where C depends on V and $\|u\|_{W^{6,\infty}}$. The price is however the dependence of C on $\|u\|_{W^{6,\infty}}$ is nonlinear.

Proof. For any $x \in \Omega_\varepsilon$, and for $i = 1, 2$, Taylor expansion at x gives

$$D_{s_i}^+ y(x) = \nabla_{s_i}^1 [y](x) + \varepsilon \nabla_{s_i}^2 [y](x) + \varepsilon^2 R_{2,s_i}[y](x),$$

where, for convenience, we have introduced the short-hands for the Taylor series and its remainder:

$$\begin{aligned} \nabla_{s_i}^j [y](x) &= \frac{1}{j!} (s_i \cdot \nabla)^j y(x), \\ R_{k,s_i}[y](x) &= \int_0^1 (k+1)(1-t)^k \nabla_{s_i}^{k+1} y(x + \varepsilon t s_i) dt, \quad k \in \mathbb{N}, \end{aligned}$$

provided that the terms on the right hand side are well defined. Obviously, we may write

$$(2.3) \quad D_{s_i}^+ = \nabla_{s_i}^1 + \varepsilon \nabla_{s_i}^2 + \varepsilon^2 R_{2,s_i}, \quad D_{s_i}^- = \nabla_{s_i}^1 - \varepsilon \nabla_{s_i}^2 - \varepsilon^2 R_{2,-s_i}.$$

For $i = 1, 2, 3$ and $t \in [0, 1]$, let

$$\begin{aligned} F_i(t) = \partial_i V_{(s_1, s_2)} &\left(|tD_{s_1}^+ y(x) + (1-t)(s_1 \cdot \nabla)y(x)|^2, \right. \\ &|tD_{s_2}^+ y(x) + (1-t)(s_2 \cdot \nabla)y(x)|^2, \\ &\langle tD_{s_1}^+ y(x) + (1-t)(s_1 \cdot \nabla)y(x), \\ &\left. tD_{s_2}^+ y(x) + (1-t)(s_2 \cdot \nabla)y(x) \rangle \right). \end{aligned}$$

Using Taylor expansion, we get

$$(2.4) \quad F_i(1) = F_i(0) + F_i'(0) + R_1[F_i](0).$$

Here for $F_i : [0, 1] \rightarrow \mathbb{R}$, we have introduced a similar short-hand for the remainder

$$R_k[F_i](0) = \int_0^1 \frac{(1-t)^k}{k!} \nabla^{k+1} F_i(t) dt.$$

Notice that by definition we have

$$\begin{aligned}
F_i(1) &= \partial_i V_{(s_1, s_2)} (|D_{s_1}^+ y(x)|^2, |D_{s_2}^+ y(x)|^2, \langle D_{s_1}^+ y(x), D_{s_2}^+ y(x) \rangle) \\
&= \partial_i V_{(s_1, s_2)} [y](x); \\
F_i(0) &= \partial_i V_{(s_1, s_2)} (|(s_1 \cdot \nabla) y(x)|^2, |(s_2 \cdot \nabla) y(x)|^2, \langle (s_1 \cdot \nabla) y(x), (s_2 \cdot \nabla) y(x) \rangle) \\
&= \partial_i W_{(s_1, s_2)} (\nabla u(x)).
\end{aligned}$$

Therefore, we can rewrite (2.4) as

$$\begin{aligned}
(2.5) \quad \partial_i V_{(s_1, s_2)} [y](x) &= \partial_i W_{(s_1, s_2)} (\nabla u(x)) + \varepsilon a_j \partial_{ij} W_{(s_1, s_2)} (\nabla u(x)) \\
&\quad + (\varepsilon^2 b_j \partial_{ij} W_{(s_1, s_2)} (\nabla u(x)) + R_1 [F_i](0)) \\
&\quad + \varepsilon^3 c_j \partial_{ij} W_{(s_1, s_2)} (\nabla u(x)) \\
&\equiv \mathcal{Q}_{i, (s_1, s_2)} [\nabla u](x),
\end{aligned}$$

where for $j = 1, 2, 3$,

$$\begin{aligned}
a_j &= 2 \left\langle (s_j \cdot \nabla) y, \nabla_{s_j}^2 [y] \right\rangle (1 - \delta_{j3}) \\
&\quad + (\left\langle (s_1 \cdot \nabla) y, \nabla_{s_2}^2 [y] \right\rangle + \left\langle (s_2 \cdot \nabla) y, \nabla_{s_1}^2 [y] \right\rangle) \delta_{j3}, \\
b_j &= 2 \left\langle (s_j \cdot \nabla) y, \nabla_{s_j}^3 [y] \right\rangle (1 - \delta_{j3}) \\
&\quad + (\left\langle (s_1 \cdot \nabla) y, \nabla_{s_2}^3 [y] \right\rangle + \left\langle (s_2 \cdot \nabla) y, \nabla_{s_1}^3 [y] \right\rangle) \delta_{j3}, \\
c_j &= 2 \left\langle (s_j \cdot \nabla) y, R_{2, s_j} [y] \right\rangle (1 - \delta_{j3}) \\
&\quad + (\left\langle (s_1 \cdot \nabla) y, R_{2, s_2} [y] \right\rangle + \left\langle (s_2 \cdot \nabla) y, R_{2, s_1} [y] \right\rangle) \delta_{j3}.
\end{aligned}$$

Substituting the equations (2.3) into $\mathcal{F}_{\text{at}}[y](x)$, we obtain

$$\begin{aligned}
\mathcal{F}_{\text{at}}[y] &= \\
&\sum_{(s_1, s_2) \in S} (\nabla_{s_1}^1 - \varepsilon \nabla_{s_1}^2 - \varepsilon^2 R_{2, -s_1}) \left\{ 2 \partial_1 V_{(s_1, s_2)} [y] (\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1}) [y] \right. \\
&\quad \left. + \partial_3 V_{(s_1, s_2)} [y] (\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2}) [y] \right\} \\
&\quad + (\nabla_{s_2}^1 - \varepsilon \nabla_{s_2}^2 - \varepsilon^2 R_{2, -s_2}) \left\{ 2 \partial_2 V_{(s_1, s_2)} [y] (\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2}) [y] \right. \\
&\quad \left. + \partial_3 V_{(s_1, s_2)} [y] (\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1}) [y] \right\}.
\end{aligned}$$

Next substituting (2.5) into the above equation, we have

$$\begin{aligned} \mathcal{F}_{\text{at}}[y](x) = & \sum_{(s_1, s_2) \in S} (\nabla_{s_1}^1 - \varepsilon \nabla_{s_1}^2 - \varepsilon^2 R_{2, -s_1}) \left\{ 2\mathcal{Q}_{1, (s_1, s_2)}[\nabla u](\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1})[y] \right. \\ & \left. + \mathcal{Q}_{3, (s_1, s_2)}[\nabla u](\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2})[y] \right\} \\ & + (\nabla_{s_2}^1 - \varepsilon \nabla_{s_2}^2 - \varepsilon^2 R_{2, -s_2}) \left\{ 2\mathcal{Q}_{2, (s_1, s_2)}[\nabla u](\nabla_{s_2}^1 + \varepsilon \nabla_{s_2}^2 + \varepsilon^2 R_{2, s_2})[y] \right. \\ & \left. + \mathcal{Q}_{3, (s_1, s_2)}[\nabla u](\nabla_{s_1}^1 + \varepsilon \nabla_{s_1}^2 + \varepsilon^2 R_{2, s_1})[y] \right\}. \end{aligned}$$

Collecting the terms of the same order, we get

$$(2.6) \quad \mathcal{F}_{\text{at}}[y](x) = \mathcal{L}_0[u](x) + \varepsilon \mathcal{L}_1[u](x) + \varepsilon^2 \mathcal{L}_2[u](x) + \mathcal{O}(\varepsilon^3).$$

If we change ε to $-\varepsilon$, the left-hand side of (2.6) is invariant, then the terms of odd power of ε in the right-hand side of (2.6) automatically vanishes. Therefore, we have

$$\mathcal{F}_{\text{at}}[y](x) = \mathcal{L}_0[u](x) + \varepsilon^2 \mathcal{L}_2[u](x) + \mathcal{O}(\varepsilon^4).$$

The explicit form of \mathcal{L}_0 can be written as

$$\begin{aligned} \mathcal{L}_0[u](x) = & -2(s_1 \cdot \nabla) [(s_1 + (s_1 \cdot \nabla)u) \partial_1 W_{(s_1, s_2)}(\nabla u(x))] \\ & - (s_1 \cdot \nabla) [(s_2 + (s_2 \cdot \nabla)u) \partial_3 W_{(s_1, s_2)}(\nabla u(x))] \\ & - 2(s_2 \cdot \nabla) [(s_2 + (s_2 \cdot \nabla)u) \partial_2 W_{(s_1, s_2)}(\nabla u(x))] \\ & - (s_2 \cdot \nabla) [(s_1 + (s_1 \cdot \nabla)u) \partial_3 W_{(s_1, s_2)}(\nabla u(x))]. \end{aligned}$$

We see that \mathcal{L}_0 is the same as the operator that appears in the Euler-Lagrangian equation of (1.7).

The proof of that \mathcal{L}_2 is of divergence form is similar. Actually, \mathcal{L}_2 is a quasilinear operator, which actually counts for the linear dependence on $\|u\|_{W^{16, \infty}}$ on the right-hand side of (2.1). To prove (2.1), it remains to estimate terms of $\mathcal{O}(\varepsilon^2)$, which is a combination of terms of the form: for $\alpha, \beta = 1, 2$,

$$\begin{aligned} & \nabla_{s_\alpha}^k \left(\partial_i W_{(s_1, s_2)}(\nabla u) \nabla_{s_\beta}^l u \right), \quad l + k = 4, l, k \in \mathbb{N}, \\ & \nabla_{s_\alpha}^k \left(a_j \partial_{ij} W_{(s_1, s_2)}(\nabla u) \nabla_{s_\beta}^l u \right), \quad l + k = 3, l, k \in \mathbb{N}, \\ & \nabla_{s_\alpha}^1 \left(b_j \partial_{ij} W_{(s_1, s_2)}(\nabla u) \nabla_{s_\beta}^1 u + R_1[F_i](0) \nabla_{s_\beta}^1 u \right). \end{aligned}$$

We only give the estimate for the first term, and the other two can be bounded similarly. Due to chain rule and to Leibniz's rule, $\nabla_{s_\alpha}^k \left(\partial_i W_{(s_1, s_2)}(\nabla u) \nabla_{s_\beta}^l u \right)$ is a

linear combination of the form

$$T = \prod_{i=1}^3 \left(\frac{\partial}{\partial x_i} \right)^{\text{sgn } \delta_i} \partial_i W_{(s_1, s_2)}(\nabla u) \\ \times (s_\alpha \cdot \nabla)^{\gamma_1} P_{\delta_1}(s_\alpha \cdot \nabla)^{\gamma_2} P_{\delta_2}(s_\alpha \cdot \nabla)^{\gamma_3} P_{\delta_3}(s_\beta \cdot \nabla)^{4-|\gamma|} u,$$

where $\gamma \in \mathbb{N}^3$ are multiindices with $|\gamma| = \sum_{i=1}^3 |\gamma_i|$ and $|\gamma| \leq 3$. Here

$$P_1 = |s_1 + (s_1 \cdot \nabla)u|^2, \quad P_2 = |s_2 + (s_2 \cdot \nabla)u|^2, \quad P_3 = \langle s_1 + (s_1 \cdot \nabla)u, s_2 + (s_2 \cdot \nabla)u \rangle.$$

Using chain rule once again, we get, for $i = 1, 2, 3$,

$$\begin{aligned} \|(s_\alpha \cdot \nabla)P_i\|_{L^\infty} &\leq C(s_\alpha)(1 + \|\nabla u\|_{L^\infty})\|\nabla^2 u\|_{L^\infty}, \\ \|(s_\alpha \cdot \nabla)^2 P_i\|_{L^\infty} &\leq C(s_\alpha) \left((1 + \|\nabla u\|_{L^\infty})\|\nabla^3 u\|_{L^\infty} + \|\nabla^2 u\|_{L^\infty}^2 \right), \\ \|(s_\alpha \cdot \nabla)^3 P_i\|_{L^\infty} &\leq C(s_\alpha) \left((1 + \|\nabla u\|_{L^\infty})\|\nabla^4 u\|_{L^\infty} + \|\nabla^2 u\|_{L^\infty}^2 \|\nabla^3 u\|_{L^\infty} \right). \end{aligned}$$

Using Gagliardo-Nirenberg inequality [32],

$$\|\nabla^j u\|_{L^\infty} \leq C \|\nabla^m u\|_{L^\infty}^{j/m} \|u\|_{L^\infty}^{1-j/m}, \quad 0 < j < m,$$

we have

$$\|(s_\alpha \cdot \nabla)^k P_i\|_{L^\infty} \leq C(s_\alpha) \left(\|u\|_{L^\infty} \|\nabla^{k+2} u\|_{L^\infty} + \|\nabla^{k+1} u\|_{L^\infty} \right).$$

Using the above inequality, we conclude

$$\begin{aligned} \|T\|_{L^\infty} &\leq C \max_{2 \leq |\gamma| \leq 4} \|\partial_\gamma W_{(s_1, s_2)}(\nabla u)\|_{L^\infty} \|\nabla^{4-|\gamma|} u\|_{L^\infty} \\ &\times \left\{ (1 + \|u\|_{L^\infty}^3) \prod_{i=1}^3 \|\nabla^{\gamma_i+2} u\|_{L^\infty} + \prod_{i=1}^3 \|\nabla^{\gamma_i+1} u\|_{L^\infty} \right. \\ &\quad + (1 + \|u\|_{L^\infty}^2) \sum_{i,j,k=1}^3 \|\nabla^{\gamma_i+2} u\|_{L^\infty} \|\nabla^{\gamma_j+2} u\|_{L^\infty} \|\nabla^{\gamma_k+1} u\|_{L^\infty} \\ &\quad \left. + (1 + \|u\|_{L^\infty}) \sum_{i,j,k=1}^3 \|\nabla^{\gamma_i+2} u\|_{L^\infty} \|\nabla^{\gamma_j+1} u\|_{L^\infty} \|\nabla^{\gamma_k+1} u\|_{L^\infty} \right\}. \end{aligned}$$

Invoking Gagliardo-Nirenberg inequality again, we obtain

$$\begin{aligned} \|T\|_{L^\infty} &\leq C(\|u\|_{L^\infty}^3 + \|u\|_{L^\infty}^6) \|\nabla^{10} u\|_{L^\infty} \\ &\quad + C(\|u\|_{L^\infty}^3 + \|u\|_{L^\infty}^5) \|\nabla^9 u\|_{L^\infty} \\ &\quad + C(\|u\|_{L^\infty}^3 + \|u\|_{L^\infty}^4) \|\nabla^8 u\|_{L^\infty} \\ &\quad + C\|u\|_{L^\infty}^3 \|\nabla^7 u\|_{L^\infty} \\ &\leq C \sum_{i=3}^6 \|u\|_{L^\infty}^i \|u\|_{W^{10,\infty}}. \end{aligned}$$

Proceeding along the same line, we can obtain the similar bounds for the higher-order terms, while $\|u\|_{W^{16,\infty}}$ arises from the following term

$$R_{\alpha,-s_\alpha} \left(\partial_i W_{(s_1,s_2)}(\nabla u) R_{\beta,s_\beta}[y] \right).$$

Summing up all terms of $\mathcal{O}(\varepsilon^2)$, we get (2.1). □

Corollary 2.2 (Consistency of finite element discretization). *For any $y = x + u(x)$ with u smooth, we have*

$$\|\mathcal{F}_\varepsilon[y] - \mathcal{F}_{\text{CB}}[y]\|_{L^\infty_\varepsilon} \leq C\varepsilon^2 \|u\|_{W^{16,\infty}},$$

where the constant C depends on V and $\|u\|_{L^\infty}$, but is independent of ε .

Proof. The corollary follows Lemma 2.1 by the observation that we can view the energy functional of the finite element discretization as a particular choice of atomistic potential energy.

To be more concrete, let us consider the case $d = 2$, so that each element $T \in \mathcal{T}_\varepsilon$ has three vertices. It is straightforward to extend the argument below to higher dimensions, with certain complication of notations.

Let $y_\varepsilon \in \tilde{X}_\varepsilon$ be the approximation of y so that $y_\varepsilon(x) = y(x)$ for any $x \in \Omega_\varepsilon$. Let $u_\varepsilon = y_\varepsilon - x$. Obviously, we have $u_\varepsilon(x) = u(x)$ for any $x \in \Omega_\varepsilon$.

Now, for each $T \in \mathcal{T}_\varepsilon$, $\nabla u_\varepsilon|_T$ is a linear function of y_ε on the vertices of T . Denote the three vertices of T as x_0, x_1, x_2 , and $s_1 = (x_1 - x_0)/\varepsilon$, $s_2 = (x_2 - x_0)/\varepsilon$, then $\nabla u_\varepsilon|_T$ is the solution of the linear system

$$\begin{cases} s_1 + s_1 A = D_{\varepsilon,s_1}^+ y_\varepsilon(x_0), \\ s_2 + s_2 A = D_{\varepsilon,s_2}^+ y_\varepsilon(x_0). \end{cases}$$

Therefore, let us denote

$$\nabla u_\varepsilon|_T = A_{(s_1,s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon)$$

as the solution of the above system. Notice that due to linearity, the map $A_{(s_1,s_2)}$ is independent of ε . Hence, for $x \in T$, we can write

$$\begin{aligned} (2.7) \quad W_{\text{CB}}(\nabla u_\varepsilon(x)) &= W_{\text{CB}}(A_{(s_1,s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon)) \\ &= W_{\text{FE},(s_1,s_2)}(y_\varepsilon(x_0)/\varepsilon, y_\varepsilon(x_1)/\varepsilon, y_\varepsilon(x_2)/\varepsilon), \end{aligned}$$

where $W_{\text{FE},(s_1,s_2)} \equiv W_{\text{CB}} \circ A_{(s_1,s_2)}$. Denote S_{FE} as the set of all pairs (s_1, s_2) such that $\{x_0, x_0 + \varepsilon s_1, x_0 + \varepsilon s_2\}$ forms the vertices of an element $T \in \mathcal{T}_\varepsilon$ containing x_0

(it is easy to see that S_{FE} is independent of ε). Then, using (2.7), we have

$$\begin{aligned}
& \int_{\Omega} W_{\text{CB}}(\nabla u_{\varepsilon}(x)) \\
&= \sum_{T \in \mathcal{T}_{\varepsilon}} |T| W_{\text{CB}}(\nabla u_{\varepsilon}|_T) \\
&= \frac{1}{3!} \sum_{x \in \Omega_{\varepsilon}} \sum_{(s_1, s_2) \in S_{\text{FE}}} \varepsilon^d |T_{(s_1, s_2)}| W_{\text{FE}, (s_1, s_2)} \left(\frac{y_{\varepsilon}(x)}{\varepsilon}, \frac{y_{\varepsilon}(x + \varepsilon s_1)}{\varepsilon}, \frac{y_{\varepsilon}(x + \varepsilon s_2)}{\varepsilon} \right) \\
&= \frac{1}{3!} \varepsilon^d \sum_{x \in \Omega_{\varepsilon}} \sum_{(s_1, s_2) \in S_{\text{FE}}} V_{\text{FE}, (s_1, s_2)} \left(\frac{y_{\varepsilon}(x)}{\varepsilon}, \frac{y_{\varepsilon}(x + \varepsilon s_1)}{\varepsilon}, \frac{y_{\varepsilon}(x + \varepsilon s_2)}{\varepsilon} \right),
\end{aligned}$$

where $V_{\text{FE}, (s_1, s_2)} = |T_{(s_1, s_2)}| W_{\text{FE}, (s_1, s_2)}$ and $T_{(s_1, s_2)}$ is the triangle formed by vectors s_1 and s_2 . This indicates that we can view the energy functional in the finite element discretization as a particular atomistic potential model, given by three body interactions $V_{\text{FE}, (s_1, s_2)}$, by identifying the value of y on nodes as the deformed atom positions.

It is immediately clear that the Cauchy-Born energy density corresponding to the atomic potential constructed is just W_{CB} . Indeed, for a homogenously deformed system with deformation gradient A , by definition, the energy of the system is just $W_{\text{CB}}(A)|\Omega|$, and hence the Cauchy-Born energy density is given again by $W_{\text{CB}}(A)$.

With this viewpoint of the finite element discretization as an atomic potential, we obtain the conclusion as an immediate corollary of Lemma 2.1. \square

Corollary 2.3 (Local truncation error). *For any $y = x + u(x)$ with u smooth, we have*

$$(2.8) \quad \|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{at}}[y]\|_{L_{\varepsilon}^{\infty}} \leq C\varepsilon^2 \|u\|_{W^{16, \infty}},$$

and

$$(2.9) \quad \|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}} \leq C\varepsilon^2 \|u\|_{W^{16, \infty}},$$

where the constant C depends on V and $\|u\|_{L^{\infty}}$, but is independent of ε .

Proof. The inequality (2.8) follows from Lemma 2.1, Corollary 2.2, and

$$\begin{aligned}
\|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{at}}[y]\|_{L_{\varepsilon}^{\infty}} &= \|\rho(x)(\mathcal{F}_{\varepsilon}[y](x) - \mathcal{F}_{\text{at}}[y](x))\|_{L_{\varepsilon}^{\infty}} \\
&\leq \|\mathcal{F}_{\varepsilon}[y] - \mathcal{F}_{\text{at}}[y]\|_{L_{\varepsilon}^{\infty}} \\
&\leq \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}} + \|\mathcal{F}_{\varepsilon}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}},
\end{aligned}$$

where we have used $\varrho(x) \in [0, 1]$. Similarly, (2.9) follows from Lemma 2.1, Corollary 2.2, and

$$\begin{aligned}
\|\mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}} &\leq \|\rho(x)(\mathcal{F}_{\varepsilon}[y](x) - \mathcal{F}_{\text{CB}}[y](x))\|_{L_{\varepsilon}^{\infty}} \\
&\quad + \|(1 - \rho(x))(\mathcal{F}_{\text{at}}[y](x) - \mathcal{F}_{\text{CB}}[y](x))\|_{L_{\varepsilon}^{\infty}} \\
&\leq \|\mathcal{F}_{\varepsilon}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}} + \|\mathcal{F}_{\text{at}}[y] - \mathcal{F}_{\text{CB}}[y]\|_{L_{\varepsilon}^{\infty}}.
\end{aligned}$$

\square

3. REGULARITY ESTIMATE

To analyze the stability property of the proposed force-based hybrid method, we use the framework of pseudo-difference operators [27, 40]. In this section, we will establish regularity estimate Theorem 3 for the force-based hybrid method. This will be one of the key ingredients used to prove stability estimate in the next section.

We study the linearized operator of \mathcal{F}_{hy} . Let us denote $\mathcal{H}_{\text{hy}}[u]$ the linearization of \mathcal{F}_{hy} at state u :

$$\mathcal{H}_{\text{hy}}[u] = \left. \frac{\delta \mathcal{F}_{\text{hy}}}{\delta y} \right|_{y=x+u},$$

so that $\mathcal{H}_{\text{hy}}[u]$ is a linear operator on lattice functions w , given by

$$\mathcal{H}_{\text{hy}}[u]w = \lim_{t \rightarrow 0} \frac{\partial \mathcal{F}_{\text{hy}}[x + u + tw]}{\partial t}.$$

It is convenient to rewrite \mathcal{H}_{hy} in the form of a pseudo-difference operator as

$$\mathcal{H}_{\text{hy}}[u] = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) T^\mu,$$

where the coefficient $h_{\text{hy}}[u](x, \mu)$ is a $d \times d$ (probably asymmetric) matrix for each x and $\mu \in \mathcal{A}$, given by

$$(3.1) \quad (h_{\text{hy}}[u])_{\alpha\beta}(x, \mu) = \left. \frac{\partial (\mathcal{F}_{\text{hy}}[y])_\alpha(x)}{\partial (T^\mu y)_\beta(x)} \right|_{y=x+u},$$

where $\alpha, \beta = 1, \dots, d$ are indices. Here \mathcal{A} is range of the pseudo-difference stencil (note that $0 \in \mathcal{A}$), which is finite by assumptions. By the definition of \mathcal{F}_{hy} , we have

$$(3.2) \quad h_{\text{hy}}[u](x, \mu) = (1 - \varrho(x)) h_{\text{at}}[u](x, \mu) + \varrho(x) h_\varepsilon[u](x, \mu),$$

where $h_{\text{at}}[u]$ and $h_\varepsilon[u]$ are given by similar equations as (3.1) by replacing \mathcal{F}_{hy} to \mathcal{F}_{at} and \mathcal{F}_ε respectively.

Define $\tilde{h}_{\text{hy}}[u](x, \xi)$ as the symbol of the pseudo-difference operator $\mathcal{H}_{\text{hy}}[u]$ given as

$$\tilde{h}_{\text{hy}}[u](x, \xi) = \sum_{\mu \in \mathcal{A}} h_{\text{hy}}[u](x, \mu) \exp(i\varepsilon \sum_j \mu_j a_j \cdot \xi) \quad \text{for } \xi \in \mathbb{L}_\varepsilon^*,$$

and similarly for $\tilde{h}_\varepsilon[u]$ and $\tilde{h}_{\text{at}}[u]$. By definition, we have for any $x \in \Omega_\varepsilon$,

$$(\mathcal{H}_{\text{hy}}[u] e_k e^{ix \cdot \xi})_j(x) = (\tilde{h}_{\text{hy}}[u])_{jk}(x, \xi) e^{ix \cdot \xi},$$

for $1 \leq j, k \leq d$ and similarly for $\tilde{h}_\varepsilon[u]$ and $\tilde{h}_{\text{at}}[u]$. Here $\{e_k\}$ are the canonical basis of \mathbb{R}^d . It is also clear that (3.2) implies

$$(3.3) \quad \tilde{h}_{\text{hy}}[u](x, \xi) = (1 - \varrho(x)) \tilde{h}_{\text{at}}[u](x, \xi) + \varrho(x) \tilde{h}_\varepsilon[u](x, \xi).$$

In the case that we linearize around the equilibrium state $u = 0$, we will simplify the notation as

$$\mathcal{H}_{\text{hy}} = \mathcal{H}_{\text{hy}}[0], \quad h_{\text{hy}} = h_{\text{hy}}[0], \quad \tilde{h}_{\text{hy}} = \tilde{h}_{\text{hy}}[0],$$

and similarly for those defined for atomistic model and finite element discretization. We observe that by the translation invariance of the total energy I_{at} at the state $u = 0$,

$$h_{\text{at}}(x, \mu) = h_{\text{at}}(\mu), \quad h_{\varepsilon}(x, \mu) = h_{\varepsilon}(\mu).$$

The coefficients are independent of position x , and hence similarly for \tilde{h}_{at} and \tilde{h}_{ε} .

We also denote \mathcal{H}_{CB} as the linearization of \mathcal{F}_{CB} at the equilibrium state $u = 0$, and define $\tilde{h}_{\text{CB}} = \tilde{h}_{\text{CB}}(x, \xi)$ as its symbol. Note that due to the periodic boundary condition assumed on Ω , ξ here only takes value in \mathbb{L}^* . Again, due to the translation invariance of the total energy, \tilde{h}_{CB} is independent of x .

Let us start the analysis with the operator \mathcal{H}_{hy} . First, we show that the matrix \tilde{h}_{hy} is Hermitian.

Lemma 3.1. *The matrices $\tilde{h}_{\text{at}}(\xi)$, $\tilde{h}_{\varepsilon}(\xi)$ and hence $\tilde{h}_{\text{hy}}(x, \xi)$ are Hermitian for any $\varepsilon > 0$, $x \in \Omega_{\varepsilon}$ and $\xi \in \mathbb{L}_{\varepsilon}^*$.*

Proof. It suffices to prove the result for $\tilde{h}_{\text{at}}(\xi)$, as the argument for $\tilde{h}_{\varepsilon}(\xi)$ is the same and the conclusion for $\tilde{h}_{\text{hy}}(x, \xi)$ follows immediately from (3.3).

Since $(\mathcal{F}_{\text{at}}[y])_{\alpha}(x) = -\partial I_{\text{at}}[y]/\partial y_{\alpha}(x)$, we have

$$\begin{aligned} (h_{\text{at}})_{\alpha\beta}(\mu) &= -\frac{\partial^2 I_{\text{at}}[y]}{\partial y_{\alpha}(x) \partial (T^{\mu}y)_{\beta}(x)} \Big|_{y=x} \\ &= -\frac{\partial^2 I_{\text{at}}[y]}{\partial y_{\alpha}(x) \partial y_{\beta}(x + \varepsilon \mu_j a_j)} \Big|_{y=x} \\ &= -\frac{\partial^2 I_{\text{at}}[y]}{\partial (T^{-\mu}y)_{\alpha}(x + \varepsilon \mu_j a_j) \partial y_{\beta}(x + \varepsilon \mu_j a_j)} \Big|_{y=x} \\ &= -\frac{\partial^2 I_{\text{at}}[y]}{\partial (T^{-\mu}y)_{\alpha}(x) \partial y_{\beta}(x)} \Big|_{y=x} = (h_{\text{at}})_{\beta\alpha}(-\mu), \end{aligned}$$

where the last line follows from translational invariance of the unperturbed system. Therefore,

$$\begin{aligned} (\tilde{h}_{\text{at}})_{\alpha\beta}(\xi) &= \sum_{\mu} (h_{\text{at}})_{\alpha\beta}(\mu) \exp(i\varepsilon \sum_j \mu_j a_j \cdot \xi) \\ &= \sum_{\mu} (h_{\text{at}})_{\beta\alpha}(-\mu) \exp(i\varepsilon \sum_j (-\mu_j) a_j \cdot (-\xi)) \\ &= \left(\sum_{\mu} (h_{\text{at}})_{\beta\alpha}(-\mu) \exp(i\varepsilon \sum_j (-\mu_j) a_j \cdot \xi) \right)^* = (\tilde{h}_{\text{at}})_{\beta\alpha}^*(\xi), \end{aligned}$$

for any $\xi \in \mathbb{L}_{\varepsilon}^*$, where we have used the fact that h_{at} are real matrices. This proves the Lemma. \square

We make the following stability assumptions about the atomistic potentials, the finite element discretization of the Cauchy-Born elasticity model:

Assumption A. $\tilde{h}_{\text{at}}(\xi)$ is positive definite and there exists $a_{\text{at}} > 0$ such that for any $\varepsilon > 0$ and any $\xi \in \mathbb{L}_\varepsilon^*$,

$$\det \tilde{h}_{\text{at}}(\xi) \geq a_{\text{at}} \Lambda_{0,\varepsilon}^{2d}(\xi).$$

Assumption B. $\tilde{h}_\varepsilon(\xi)$ is positive definite and there exists $a > 0$ such that for any $\varepsilon > 0$ and any $\xi \in \mathbb{L}_\varepsilon^*$,

$$\det \tilde{h}_\varepsilon(\xi) \geq a \Lambda_{0,\varepsilon}^{2d}(\xi).$$

The Assumptions A and B will be assumed in the sequel without further indication.

Remark. These assumptions are quite natural and physical. In fact, Assumption A is just the phonon stability conditions (for simple Bravais lattice) identified in [19] represented using the notions of pseudo-difference operators. Assumption B is the usual stability condition of a finite element discretization of continuous problem derived from the Cauchy-Born rule. We note that as a consequence of these stability assumptions, the continuous Cauchy-Born elasticity problem is also elliptic, as indicated by Corollary 4.3 below. From a mathematical point of view, Assumption A and Assumption B can be seen as the uniform ellipticity of the difference operator.

Next, we prove a lower bound for the symbol \tilde{h}_{hy} , which is crucial for the regularity and stability estimates. Let us recall an inequality proved by Ky Fan:

Theorem 2 (Ky Fan's determinant inequality [23]). *Let A, B be positive definite matrices, then for any $\lambda \in [0, 1]$,*

$$\det(\lambda A + (1 - \lambda)B) \geq (\det A)^\lambda (\det B)^{1-\lambda}.$$

Corollary 3.2. *For any $\varepsilon > 0$, $x \in \Omega_\varepsilon$ and any $\xi \in \mathbb{L}_\varepsilon^*$, we have*

$$\det \tilde{h}_{\text{hy}}(x, \xi) \geq \min(a, a_{\text{at}}) \Lambda_{0,\varepsilon}^{2d}(\xi).$$

Proof. This is an immediate corollary of Theorem 2. Since for any x , $\varrho(x) \in [0, 1]$, we have

$$\begin{aligned} \det \tilde{h}_{\text{hy}}(x, \xi) &= \det((1 - \varrho(x))\tilde{h}_{\text{at}}(\xi) + \varrho(x)\tilde{h}_\varepsilon(\xi)) \\ &\geq (\det \tilde{h}_{\text{at}}(\xi))^{1-\varrho(x)} (\det \tilde{h}_\varepsilon(\xi))^{\varrho(x)} \\ &\geq a_{\text{at}}^{1-\varrho(x)} a^{\varrho(x)} \Lambda_{0,\varepsilon}^{2d}(\xi) \\ &\geq \min(a, a_{\text{at}}) \Lambda_{0,\varepsilon}^{2d}(\xi). \end{aligned}$$

□

With these preparations, we now establish the regularity estimate of the quasi-continuum approximation. The regularity of discrete elliptic systems is understood

by a fundamental result of finite difference approximation by Bube and Strikwerda [9]. They extended the regularity estimate of Thomée and Westergren [39] from single elliptic equation to elliptic systems.

Let us introduce the regular discrete elliptic system following [9]. The concept is parallel to the regular continuous elliptic system [1].

Definition 3.3 (Regular discrete elliptic system). For $i, j = 1, \dots, d$, let L_{ij} be a difference operator with symbol $l_{ij}(x, \xi)$. The system of difference equations

$$(3.4) \quad \sum_{j=1}^d L_{ij} v_j(x) = f_i(x), \quad i = 1, \dots, d,$$

is a *regular discrete elliptic system*, if there are set of integers $\{\sigma_i\}_{i=1}^d$ and $\{\tau_j\}_{j=1}^d$ such that each L_{ij} is a difference operator of order at most $\sigma_i + \tau_j$, and if there are positive constants C, ξ_0, ε_0 such that

$$|\det l_{ij}(x, \xi)| \geq C \Lambda_\varepsilon^{2p}(\xi)$$

for $0 < \varepsilon \leq \varepsilon_0$, $\xi \in \mathbb{L}_\varepsilon^*$, and $\max_{1 \leq i \leq d} |\xi_i| \geq \xi_0$, where $2p = \sum_i (\sigma_i + \tau_i)$. We will say that the system (3.4) is regular elliptic of order (σ, τ) .

By Corollary 3.2, we immediately have

Proposition 3.4. *Under Assumptions A and B, the finite difference system*

$$(3.5) \quad \mathcal{H}_{\text{hy}} v = f$$

is a regular discrete elliptic system of order $(0, 2)$.

For the regular discrete elliptic system (3.5), we have the following regularity estimate.

Theorem 3. *Under Assumptions A and B, for any $v \in H_\varepsilon^2(\Omega)$, we have*

$$(3.6) \quad \|v\|_{\varepsilon, 2} \leq C(\|\mathcal{H}_{\text{hy}} v\|_{\varepsilon, 0} + \|v\|_{\varepsilon, 0}).$$

The constant C is independent of v and ε .

Remark. Theorem 3 is analogous to the interior regularity estimate for elliptic partial differential equations given in [2]. The statement of the theorem is just rewriting Theorem 2.1 in [9] using the current notation. We note that in [9], Bube and Strikwerda proved interior regularity estimates, which clearly implies the *a priori* estimate for periodic case here.

4. STABILITY

The main theorem we will prove in this section is the following stability estimate.

Theorem 4 (Stability). *Under Assumptions A and B, for any $v \in H_\varepsilon^2(\Omega)$, we have*

$$(4.1) \quad \|v\|_{\varepsilon, 2} \leq C \|\mathcal{H}_{\text{hy}} v\|_{\varepsilon, 0}.$$

Let us make some remarks about the stability result. In general, we do not know whether a stability estimate like (4.1) is valid for the force-based quasicontinuum method in general dimension (see [11, 14] for some study in one dimension). From a pseudo-difference operator point of view, the continuity in x variable of the symbol of the linearized operator is crucial for the validity of the strong stability. This is also the main motivation to use a smooth transition function $\varrho(x)$ in the current scheme. The strong stability property of the scheme will facilitate the numerical solution based on iterative methods.

We also note that the strong stability is also crucial for the extension of the current scheme to the time-dependent case. It plays the role of Gårding inequality. We will leave this to future publications.

To obtain the stability estimate from the regularity estimate of Theorem 3, we need to eliminate $\|v\|_{\varepsilon,0}$ on the right hand side of (3.6). In spatial dimension one, this can be achieved by the discrete maximum principle for the finite difference equation. This is however no longer the case for higher dimensions, as then we are dealing with an elliptic system. The argument we will use is instead similar in spirit to the argument used in [1, 34] for passing from regularity estimate to uniqueness results for elliptic systems.

The difficulty however is that a compactness argument as in [34] can not apply to the finite difference system, as we need a uniform estimate for different ε . Therefore, instead of using the compactness, the proof is based on the uniqueness of the continuous system from ellipticity, the consistency of the finite difference schemes to the continuous system, and the regularity estimate Theorem 3. We note that a similar approach was considered by Martin [28].

In order to connect the finite difference system with continuous PDE, we need to extend grid functions on Ω_ε to continuous functions defined in Ω . For this purpose, let us define an interpolation operator Q_ε as follows.¹ For any lattice function u on Ω_ε , we define $Q_\varepsilon u \in L^2(\Omega)$ as

$$(4.2) \quad (Q_\varepsilon u)(x) = (2\pi)^{d/2} \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \hat{u}(\xi), \quad x \in \Omega.$$

Comparing with (1.2), we know that $Q_\varepsilon u$ agrees with u on Ω_ε . We have the following properties of Q_ε .

Lemma 4.1. *For $k \geq 0$, there exists constants $c_k, C_k > 0$, such that for any u ,*

$$c_k \|u\|_{H_\varepsilon^k(\Omega)} \leq \|Q_\varepsilon u\|_{H^k(\Omega)} \leq C_k \|u\|_{H_\varepsilon^k(\Omega)}.$$

Proof. The conclusion follows immediately from definition (4.2) and (1.3). \square

¹ Usual linear interpolations are not sufficient for our purpose as we need high regularity of the interpolated functions.

Let χ be a standard nonnegative cut-off function on \mathbb{R}^d , which is smooth and compactly supported, with $\|\chi\|_{L^1} = 1$. Let χ_ε be the scaled version

$$\chi_\varepsilon(x) = \varepsilon^{-(\alpha d)} \chi(\varepsilon^{-\alpha} x),$$

for some α with $0 < \alpha < 1$. The choice of the value of α will be specified later in the proof of Proposition 4.4.

Define a low-pass filter operator L_ε for $f \in L^2(\Omega)$ using $\widehat{\chi_\varepsilon}$ as Fourier multiplier:

$$\widehat{L_\varepsilon f}(\xi) = (2\pi)^{d/2} \widehat{f}(\xi) \widehat{\chi_\varepsilon}(\xi) = (2\pi)^{d/2} \widehat{f}(\xi) \widehat{\chi}(\varepsilon^\alpha \xi).$$

In real space, L_ε convolves f with χ_ε . Note that, using integration by parts, it is easy to see that

$$(4.3) \quad |\widehat{\chi_\varepsilon}(\xi)| \leq C_k |\varepsilon^\alpha \xi|^{-k}, \quad \forall k \in \mathbb{Z}_+,$$

$$(4.4) \quad (2\pi)^{d/2} \widehat{\chi_\varepsilon}(0) = 1.$$

Hence, L_ε is indeed a low-pass filter. For simplicity of notation, we will denote

$$\overline{u}_\varepsilon = L_\varepsilon Q_\varepsilon u_\varepsilon,$$

for lattice function u_ε on Ω_ε .

We state and prove a consistency result for the linearized operator in terms of symbols.

Proposition 4.2 (Consistency of linearized operator). *There exists $\varepsilon_0 > 0$ and $s > 0$ such that for any $\varepsilon \leq \varepsilon_0$ and $\xi, \eta \in \mathbb{L}_\varepsilon^*$, we have*

$$|\widehat{h}_{\text{CB}}(\xi, \eta) - \widehat{h}_{\text{hy}}(\xi, \eta)| \leq C\varepsilon^2(|\eta| + 1)^s.$$

Proof. By definition, for $1 \leq j, k \leq d$,

$$\begin{aligned} (\widehat{h}_{\text{hy}})_{jk}(\xi, \eta) &= \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} (\widetilde{h}_{\text{hy}})_{jk}(x, \eta) \\ &= \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i(\xi + \eta) \cdot x} (\mathcal{H}_{\text{hy}}(e_k f_\eta))_j(x). \end{aligned}$$

where $f_\eta(x) = e^{i x \cdot \eta}$ for $x \in \Omega$ and

$$\begin{aligned} (\widehat{h}_{\text{CB}})_{jk}(\xi, \eta) &= (2\pi)^{-d/2} \int_{\Omega} e^{-i\xi \cdot x} dx (\widetilde{h}_{\text{CB}})_{jk}(\eta) \\ &= \varepsilon^d (2\pi)^{d/2} \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} (\widetilde{h}_{\text{CB}})_{jk}(\eta) \\ &= \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i(\xi + \eta) \cdot x} (\mathcal{H}_{\text{CB}}(e_k f_\eta))_j(x), \end{aligned}$$

where we have used in the fact that $\widetilde{h}_{\text{CB}}(x, \eta) = \widetilde{h}_{\text{CB}}(\eta)$ due to translational symmetry. Note that we get from the second line from the first line in the above equation using the fact that ξ takes value in \mathbb{L}_ε^* , so that the integral equals to the sum.

Hence, taking difference of the above two equations, we obtain the bound

$$|\widehat{h}_{\text{hy}}(\xi, \eta) - \widehat{h}_{\text{CB}}(\xi, \eta)| \leq C \sup_{1 \leq k \leq d} \|\mathcal{H}_{\text{hy}}(e_k f_\eta) - \mathcal{H}_{\text{CB}}(e_k f_\eta)\|_{L_\varepsilon^\infty}.$$

Note that by the definition of linearized operators \mathcal{H}_{hy} and \mathcal{H}_{CB} , we have

$$\mathcal{H}_{\text{hy}}(e_k f_\eta) - \mathcal{H}_{\text{CB}}(e_k f_\eta) = \lim_{t \rightarrow 0^+} \frac{1}{t} (\mathcal{F}_{\text{hy}}[x + t(e_k f_\eta)] - \mathcal{F}_{\text{CB}}[x + t(e_k f_\eta)]).$$

Hence,

$$\begin{aligned} \|\mathcal{H}_{\text{hy}}(e_k f_\eta) - \mathcal{H}_{\text{CB}}(e_k f_\eta)\|_{L_\varepsilon^\infty} &= \lim_{t \rightarrow 0^+} \frac{1}{t} \|\mathcal{F}_{\text{hy}}[x + t(e_k f_\eta)] - \mathcal{F}_{\text{CB}}[x + t(e_k f_\eta)]\|_{L_\varepsilon^\infty} \\ &\leq C\varepsilon^2 \|e_k f_\eta\|_{W^{16, \infty}} \leq C\varepsilon^2 \|e_k f_\eta\|_{H^s} \leq C\varepsilon^2 (1 + |\eta|)^s, \end{aligned}$$

where s is chosen so that the Sobolev inequality

$$\|f\|_{W^{16, \infty}(\Omega)} \leq C \|f\|_{H^s(\Omega)}$$

holds for any $f \in H^s(\Omega)$ (s depends on the dimension). Here, we have used Corollary 2.3, noticing that $\|te_k f_\eta\|_{L^\infty}$ is uniformly bounded for η as $t \rightarrow 0$. This concludes the proof. \square

The proof of Proposition 4.2 actually gives for any $\varepsilon \leq \varepsilon_0$, $x \in \Omega_\varepsilon$ and $\eta \in \mathbb{L}_\varepsilon^*$,

$$(4.5) \quad |\widetilde{h}_{\text{hy}}(x, \eta) - \widetilde{h}_{\text{CB}}(\eta)| \leq C\varepsilon^2 (1 + |\eta|)^s.$$

Combined with Corollary 3.2, we get as a corollary

Corollary 4.3. *$\widetilde{h}_{\text{CB}}(\xi)$ is positive definite and there exists $a_{\text{CB}} > 0$ such that for any $\xi \in \mathbb{L}^*$,*

$$\det \widetilde{h}_{\text{CB}}(\xi) \geq a_{\text{CB}} \Lambda_0^{2d}(\xi).$$

Proof. Fixed $\xi \in \mathbb{L}^*$, take ε_1 sufficiently small, so that for $\varepsilon < \varepsilon_1$, $\xi \in \mathbb{L}_\varepsilon^*$ (it suffices to take ε_1 so small that $\varepsilon_1 \xi \in \Gamma^*$). Without loss of generality, we can take ε_1 less than ε_0 in Proposition 4.2.

From the continuous dependence of matrix determinants on matrix elements, we get from (4.5) that for any $\varepsilon \leq \varepsilon_1$ sufficiently small, $x \in \Omega_\varepsilon$

$$|\det \widetilde{h}_{\text{hy}}(x, \xi) - \det \widetilde{h}_{\text{CB}}(\xi)| \leq C\varepsilon^2 (1 + |\xi|)^s.$$

Combining the last inequality with Corollary 3.2, we get the desired estimate by taking $\varepsilon \rightarrow 0$. \square

With these preparations, let us now state the key proposition will be used in the proof of Theorem 4.

Proposition 4.4. *For $\{v_\varepsilon\}_{\varepsilon > 0}$ that $v_\varepsilon \in H_\varepsilon^2(\Omega)$ and $\|v_\varepsilon\|_{\varepsilon, 2}$ is uniformly bounded, we have*

$$(4.6) \quad \lim_{\varepsilon \rightarrow 0^+} \|\mathcal{H}_{\text{CB}} \overline{v_\varepsilon} - \overline{\mathcal{H}_{\text{hy}} v_\varepsilon}\|_{L^2(\Omega)} = 0.$$

Assume the validity of Proposition 4.4, which we will come back in the end of this section, the proof of Theorem 4 follows a *reductio ad absurdum*.

Proof of Theorem 4. Suppose (4.1) does not hold, then there is a sequence of functions $\{w_k\}$ and $\varepsilon_k > 0$ such that

$$\begin{aligned} \|w_k\|_{\varepsilon_k, 2} &\rightarrow \infty, & \text{as } k \rightarrow \infty; \\ \|\mathcal{H}_{\text{hy}} w_k\|_{\varepsilon_k, 0} &\leq c, & \text{for all } k; \\ \sum_{x \in \Omega_{\varepsilon_k}} w_k(x) &= 0, & \text{for all } k. \end{aligned}$$

Set $v_k = w_k / \|w_k\|_{\varepsilon_k, 2}$, we then have

$$\begin{aligned} (4.7) \quad \|v_k\|_{\varepsilon_k, 2} &= 1 & \text{for all } k; \\ (4.8) \quad \|\mathcal{H}_{\text{hy}} v_k\|_{\varepsilon_k, 0} &\rightarrow 0, & \text{as } k \rightarrow \infty; \\ (4.9) \quad \sum_{x \in \Omega_{\varepsilon_k}} v_k(x) &= 0, & \text{for all } k. \end{aligned}$$

Since

$$\mathcal{H}_{\text{CB}} \bar{v}_k = \overline{\mathcal{H}_{\text{hy}} v_k} + (\mathcal{H}_{\text{CB}} \bar{v}_k - \overline{\mathcal{H}_{\text{hy}} v_k}).$$

Since $\|\mathcal{H}_{\text{hy}} v_k\|_{\varepsilon_k, 0} \rightarrow 0$, we have

$$\|\overline{\mathcal{H}_{\text{hy}} v_k}\|_{L^2(\Omega)} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

Moreover, by Proposition 4.4,

$$\|\mathcal{H}_{\text{CB}} \bar{v}_k - \overline{\mathcal{H}_{\text{hy}} v_k}\|_{L^2(\Omega)} \rightarrow 0, \quad \text{as } k \rightarrow \infty.$$

Hence $\|\mathcal{H}_{\text{CB}} \bar{v}_k\|_{L^2(\Omega)} \rightarrow 0$. Note also that the average of \bar{v}_k is zero, since $\widehat{\bar{v}_k}(0) = 0$. By the invertibility of \mathcal{H}_{CB} on the subspace orthogonal to constant function, $\|\bar{v}_k\|_{L^2(\Omega)} \rightarrow 0$, as $k \rightarrow \infty$, while $\|v_k\|_{\varepsilon_k, 2} = 1$. It follows then $\|v_k\|_{\varepsilon_k, 0} \rightarrow 0$. Indeed, since

$$\|v_k\|_{\varepsilon_k, 1} = \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*} \Lambda_{\varepsilon_k}^2(\xi) |\widehat{v_k}(\xi)|^2 \leq 1,$$

for any $\delta > 0$, there exist $\Xi > 0$ and k_1 , such that for any $k \geq k_1$,

$$(4.10) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| \geq \Xi} |\widehat{v_k}(\xi)|^2 < \delta/2.$$

On the other hand, due to (4.4), there exists k_2 , such that for $k \geq k_2$

$$(4.11) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| < \Xi} ||\widehat{v_k}(\xi)|^2 - |\widehat{\bar{v}_k}(\xi)|^2| \leq \delta/4.$$

Moreover, as $\|\bar{v}_k\|_{L^2} \rightarrow 0$, there exists k_3 , such that for $k \geq k_3$,

$$(4.12) \quad \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*, |\xi| < \Xi} |\widehat{\bar{v}_k}(\xi)|^2 \leq \delta/4.$$

Combined (4.10)–(4.12) together, we have for $k \geq \max(k_1, k_2, k_3)$,

$$\|v_k\|_{\varepsilon_k,0}^2 = \sum_{\xi \in \mathbb{L}_{\varepsilon_k}^*} |\widehat{v}_k|^2 \leq \delta.$$

Hence, $\lim_{k \rightarrow \infty} \|v_k\|_{\varepsilon_k,0} = 0$. From Theorem 3, this implies

$$\lim_{k \rightarrow \infty} \|v_k\|_{\varepsilon_k,2} = 0.$$

The contradiction with the choice of v_k proves the Theorem. \square

Using perturbation, we may extend the results of Theorem 4 to a deformed state u .

Theorem 5 (Stability). *Under Assumption A and B, there exists $\delta > 0$, such that for any $\varepsilon > 0$ and u , $\|u\|_{W_\varepsilon^{2,\infty}} \leq \delta$ and any $v \in H_\varepsilon^2(\Omega)$, we have*

$$(4.13) \quad \|v\|_{\varepsilon,2} \leq C \|\mathcal{H}_{\text{hy}}[u]v\|_{\varepsilon,0},$$

where the constant depends on δ , but is independent of u , v and ε .

Proof. This theorem follows from a perturbation argument of Theorem 4. Denote by v_0 the solution of

$$\mathcal{H}_{\text{hy}}[0]v_0 = f.$$

We immediately have

$$\mathcal{H}_{\text{hy}}[0](v - v_0) = (\mathcal{H}_{\text{hy}}[0] - \mathcal{H}_{\text{hy}}[u])v.$$

Using Theorem 4, we have

$$\|v - v_0\|_{\varepsilon,2} \leq C \|(\mathcal{H}_{\text{hy}}[0] - \mathcal{H}_{\text{hy}}[u])v\|_{\varepsilon,0} \leq C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2}.$$

By triangular inequality, we have

$$\begin{aligned} \|v\|_{\varepsilon,2} &\leq \|v_0\|_{\varepsilon,2} + \|v - v_0\|_{\varepsilon,2} \\ &\leq C \|\mathcal{H}_{\text{hy}}[0]v_0\|_{\varepsilon,0} + C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2} \\ &= C \|\mathcal{H}_{\text{hy}}[u]v\|_{\varepsilon,0} + C \|\nabla u\|_{W_\varepsilon^{1,\infty}} \|v\|_{\varepsilon,2} \\ &\leq C \|\mathcal{H}_{\text{hy}}[u]v\|_{\varepsilon,0} + C\delta \|v\|_{\varepsilon,2}, \end{aligned}$$

which gives (4.13) by choosing $\delta = 1/(2C)$. \square

We conclude this section with the proof of Proposition 4.4.

Proof of Proposition 4.4. We work in the Fourier domain. By definition,

$$(\mathcal{H}_{\text{CB}} \overline{v}_\varepsilon)(x) = \sum_{\xi \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \xi} \widetilde{h}_{\text{CB}}(x, \xi) \widehat{\chi}(\varepsilon^\alpha \xi) \widehat{v}_\varepsilon(\xi).$$

Hence, taking Fourier transform,

$$\begin{aligned}\widehat{\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon}(\xi) &= (2\pi)^{-d/2} \int_{\Omega} e^{-i\xi \cdot x} \sum_{\eta \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \eta} \widetilde{h_{\text{CB}}}(x, \eta) \widehat{\chi}(\varepsilon^\alpha \eta) \widehat{v}_\varepsilon(\eta) \, dx \\ &= \sum_{\eta \in \mathbb{L}_\varepsilon^*} \widehat{h_{\text{CB}}}(\xi - \eta, \eta) \widehat{\chi}(\varepsilon^\alpha \eta) \widehat{v}_\varepsilon(\eta),\end{aligned}$$

where

$$\widehat{h_{\text{CB}}}(\xi, \eta) = (2\pi)^{-d/2} \int_{\Omega} e^{-i\xi \cdot x} \widetilde{h_{\text{CB}}}(x, \eta) \, dx$$

is the Fourier transform of the symbol with respect to x .

On the other hand, for the discrete system, we have

$$\begin{aligned}\widehat{\mathcal{H}_{\text{hy}}v_\varepsilon}(\xi) &= \widehat{\chi}(\varepsilon^\alpha \xi) \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} \sum_{\eta \in \mathbb{L}_\varepsilon^*} e^{ix \cdot \eta} \widetilde{h_{\text{hy}}}(x, \eta) \widehat{v}_\varepsilon(\eta) \\ &= \widehat{\chi}(\varepsilon^\alpha \xi) \sum_{\eta \in \mathbb{L}_\varepsilon^*} \widehat{h_{\text{hy}}}(\xi - \eta, \eta) \widehat{v}_\varepsilon(\eta),\end{aligned}$$

where

$$\widehat{h_{\text{hy}}}(\xi, \eta) = \varepsilon^d (2\pi)^{-d/2} \sum_{x \in \Omega_\varepsilon} e^{-i\xi \cdot x} \widetilde{h_{\text{hy}}}(x, \eta).$$

Let us compare the difference between $\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon$ and $\overline{\mathcal{H}_{\text{hy}}v_\varepsilon}$. We write

$$\begin{aligned}& \left| \widehat{\mathcal{H}_{\text{CB}}\bar{v}_\varepsilon}(\xi) - \widehat{\overline{\mathcal{H}_{\text{hy}}v_\varepsilon}}(\xi) \right| \\ &= \left| \sum_{\eta \in \mathbb{L}_\varepsilon^*} \left(\widehat{\chi}(\varepsilon^\alpha \eta) \widehat{h_{\text{CB}}}(\xi - \eta, \eta) - \widehat{\chi}(\varepsilon^\alpha \xi) \widehat{h_{\text{hy}}}(\xi - \eta, \eta) \right) \widehat{v}_\varepsilon(\eta) \right| \\ &\leq |\widehat{I}_1(\xi)| + |\widehat{I}_2(\xi)|,\end{aligned}$$

where

$$\begin{aligned}\widehat{I}_1(\xi) &= \sum_{\eta \in \mathbb{L}_\varepsilon^*} (\widehat{\chi}(\varepsilon^\alpha \xi) - \widehat{\chi}(\varepsilon^\alpha \eta)) \widehat{h_{\text{CB}}}(\xi - \eta, \eta) \widehat{v}_\varepsilon(\eta), \\ \widehat{I}_2(\xi) &= \widehat{\chi}(\varepsilon^\alpha \xi) \sum_{\eta \in \mathbb{L}_\varepsilon^*} (\widehat{h_{\text{CB}}}(\xi - \eta, \eta) - \widehat{h_{\text{hy}}}(\xi - \eta, \eta)) \widehat{v}_\varepsilon(\eta).\end{aligned}$$

It suffices to prove that L^2 norms of I_1 and I_2 both go to zero as $\varepsilon \rightarrow 0$. Let us estimate I_1 first. By the smoothness of χ , we have $|\widehat{\chi}(\varepsilon^\alpha \xi) - \widehat{\chi}(\varepsilon^\alpha \eta)| \leq C\varepsilon^\alpha |\xi - \eta|$, hence

$$|\widehat{I}_1(\xi)| \leq C\varepsilon^\alpha \sum_{\eta \in \mathbb{L}_\varepsilon^*} |\xi - \eta| |\Lambda^{-2}(\eta) \widehat{h_{\text{CB}}}(\xi - \eta, \eta)| |\Lambda^2(\eta) \widehat{v}_\varepsilon(\eta)|.$$

Define $\theta(\xi)$ as

$$\theta(\xi) = |\xi| \sup_{\eta \in \mathbb{L}^*} |\Lambda^{-2}(\eta) \widehat{h_{\text{CB}}}(\xi, \eta)|.$$

By the smoothness of $\widetilde{h_{\text{CB}}}(x, \xi)$ with respect to x and the fact that \mathcal{H}_{CB} is a second order operator, we have $|\xi \Lambda^{-2}(\eta) \widehat{h_{\text{CB}}}(\xi, \eta)| \leq C|\xi|^{-d-1}$ uniformly in η . Hence,

$\theta \in l^1(\mathbb{L}^*)$ as a function of ξ . Therefore,

$$\begin{aligned} \|I_1\|_{L^2(\Omega)} &= \|\widehat{I}_1\|_{l^2(\mathbb{L}^*)} \leq C\varepsilon^\alpha \|\theta\|_{l^1(\mathbb{L}^*)} \left(\sum_{\eta \in \mathbb{L}_\varepsilon^*} \Lambda^4(\eta) |\widehat{v}_\varepsilon(\eta)|^2 \right)^{1/2} \\ &\leq C\varepsilon^\alpha \|\theta\|_{l^1(\mathbb{L}^*)} \|Q_\varepsilon v_\varepsilon\|_{H^2(\Omega)} \\ &\leq C\varepsilon^\alpha \|\theta\|_{l^1(\mathbb{L}^*)} \|v_\varepsilon\|_{H_\varepsilon^2(\Omega)}, \end{aligned}$$

where the first inequality results from Young's inequality. This proves that $\|I_1\|_{L^2(\Omega)}$ goes to zero as $\varepsilon \rightarrow 0$.

Let us consider I_2 next. Take $\alpha_1 \in (\alpha, 1)$, we break I_2 into three parts

$$\widehat{I}_2(\xi) = \widehat{I}_{21}(\xi) + \widehat{I}_{22}(\xi) + \widehat{I}_{23}(\xi),$$

where

$$\begin{aligned} \widehat{I}_{21}(\xi) &= 1_{|\xi| \geq \pi\varepsilon^{-\alpha_1}} \widehat{\chi}(\varepsilon^\alpha \xi) \sum_{\eta \in \mathbb{L}_\varepsilon^*} (\widehat{h}_{\text{CB}}(\xi - \eta, \eta) - \widehat{h}_{\text{hy}}(\xi - \eta, \eta)) \widehat{v}_\varepsilon(\eta), \\ \widehat{I}_{22}(\xi) &= 1_{|\xi| < \pi\varepsilon^{-\alpha_1}} \widehat{\chi}(\varepsilon^\alpha \xi) \sum_{\substack{\eta \in \mathbb{L}_\varepsilon^*, \\ |\eta| \geq 2\pi\varepsilon^{-\alpha_1}}} (\widehat{h}_{\text{CB}}(\xi - \eta, \eta) - \widehat{h}_{\text{hy}}(\xi - \eta, \eta)) \widehat{v}_\varepsilon(\eta), \\ \widehat{I}_{23}(\xi) &= 1_{|\xi| < \pi\varepsilon^{-\alpha_1}} \widehat{\chi}(\varepsilon^\alpha \xi) \sum_{\substack{\eta \in \mathbb{L}_\varepsilon^*, \\ |\eta| < 2\pi\varepsilon^{-\alpha_1}}} (\widehat{h}_{\text{CB}}(\xi - \eta, \eta) - \widehat{h}_{\text{hy}}(\xi - \eta, \eta)) \widehat{v}_\varepsilon(\eta). \end{aligned}$$

We will control each term: I_{21} is small due to the decay property of $\widehat{\chi}$; I_{22} is small since ξ and η is well separated; I_{23} is small due to consistency.

I_{21} : Define w given by

$$\widehat{w}(\xi) = \sum_{\eta \in \mathbb{L}_\varepsilon^*} (\widehat{h}_{\text{CB}}(\xi - \eta, \eta) - \widehat{h}_{\text{hy}}(\xi - \eta, \eta)) \widehat{v}_\varepsilon(\eta).$$

We observe that $\widehat{w}(\xi)$ is the Fourier transform of

$$w(x) = (\mathcal{H}_{\text{CB}} Q_\varepsilon v_\varepsilon)(x) - (Q_\varepsilon(\mathcal{H}_{\text{hy}} v_\varepsilon))(x).$$

Hence, $\|w\|_{L^2(\Omega)} \leq C\|v_\varepsilon\|_{\varepsilon, 2}$. By (4.3), we have

$$|\widehat{\chi}(\varepsilon^\alpha \xi)| \leq C_k \varepsilon^{k(\alpha_1 - \alpha)}, \quad \forall |\xi| \geq \pi\varepsilon^{-\alpha_1},$$

for any positive integer k . Therefore, we conclude that $\|I_{21}\|_{L^2(\Omega)} \rightarrow 0$ as

$$\widehat{I}_{21}(\xi) = 1_{|\xi| \geq \pi\varepsilon^{-\alpha_1}} \widehat{\chi}(\varepsilon^\alpha \xi) \widehat{w}(\xi).$$

I_{22} : We have

$$\begin{aligned} (4.14) \quad |\widehat{I}_{22}(\xi)| &\leq C \sum_{\eta \in \mathbb{L}_\varepsilon^*} |\Lambda^{-2}(\eta) \widehat{h}_{\text{CB}}(\xi - \eta, \eta)| |\Lambda^2(\eta) \widehat{v}_\varepsilon(\eta)| 1_{|\xi - \eta| > \pi\varepsilon^{-\alpha_1}} \\ &\quad + C \sum_{\eta \in \mathbb{L}_\varepsilon^*} |\Lambda^{-2}(\varepsilon, \eta) \widehat{h}_{\text{hy}}(\xi - \eta, \eta)| |\Lambda_\varepsilon^2(\eta) \widehat{v}_\varepsilon(\eta)| 1_{|\xi - \eta| > \pi\varepsilon^{-\alpha_1}}. \end{aligned}$$

The argument for the two terms are analogous, and let us focus on the first term. Consider $\varphi(\xi)$ given by

$$\varphi(\xi) = \sup_{\eta \in \mathbb{L}^*} |\Lambda^{-2}(\eta) \hat{h}_{\text{CB}}(\xi, \eta)|.$$

Since $\tilde{h}_{\text{CB}}(x, \eta)$ is smooth with respect to x and \mathcal{H}_{CB} is a second-order operator, we have $\varphi \in l^1(\mathbb{L}^*)$ as a function of ξ . Hence

$$\lim_{\varepsilon \rightarrow 0} \|\varphi(\xi) 1_{|\xi| > \pi \varepsilon^{-\alpha_1}}\|_{l^1(\mathbb{L}^*)} = 0.$$

Therefore, using Young's inequality, the first term on the right hand side of (4.14) is bounded by $C \|\varphi(\xi) 1_{|\xi| > \pi \varepsilon^{-\alpha_1}}\|_{l^1(\mathbb{L}^*)} \|Q_\varepsilon v_\varepsilon\|_{H^2(\Omega)}$, which goes to zero as $\varepsilon \rightarrow 0$. Hence, I_{22} goes to zero in L^2 norm.

I_{23} : From Proposition 4.2, we have

$$|\hat{h}_{\text{CB}}(\xi, \eta) - \hat{h}_{\text{hy}}(\xi, \eta)| \leq C \varepsilon^2 (|\eta| + 1)^t$$

for some $s \geq 0$. As $|\eta| < 2\pi \varepsilon^{-\alpha_1}$, we have

$$|\hat{h}_{\text{CB}}(\xi, \eta) - \hat{h}_{\text{hy}}(\xi, \eta)| \leq C \varepsilon^{(2-s\alpha_1)}.$$

Therefore,

$$\begin{aligned} \sum_{\xi \in \mathbb{L}^*} |\widehat{I_{23}}(\xi)|^2 &\leq C \sum_{\substack{\xi \in \mathbb{L}^*, \\ |\xi| < \pi \varepsilon^{-\alpha_1}}} \left(\sum_{\substack{\eta \in \mathbb{L}_\varepsilon^*, \\ |\eta| < 2\pi \varepsilon^{-\alpha_1}}} (\hat{h}_{\text{CB}}(\xi - \eta, \eta) - \hat{h}_{\text{hy}}(\xi - \eta, \eta)) \hat{v}_\varepsilon(\eta) \right)^2 \\ &\leq C \sum_{\substack{\eta \in \mathbb{L}_\varepsilon^*, \\ |\eta| < 2\pi \varepsilon^{-\alpha_1}}} |\hat{v}_\varepsilon(\eta)|^2 \sum_{\substack{\xi \in \mathbb{L}^*, \\ |\xi| < \pi \varepsilon^{-\alpha_1}}} |\hat{h}_{\text{CB}}(\xi - \eta, \eta) - \hat{h}_{\text{hy}}(\xi - \eta, \eta)|^2 \\ &\leq C \varepsilon^{4-(2s+d)\alpha_1} \sum_{\substack{\eta \in \mathbb{L}_\varepsilon^*, \\ |\eta| < 2\pi \varepsilon^{-\alpha_1}}} |\hat{v}_\varepsilon(\eta)|^2. \end{aligned}$$

Hence, by choosing α_1 (and also α) sufficiently small that $\alpha_1 < 4/(2s+d)$, we have $\|I_{23}\|_{L^2} \rightarrow 0$ as $\varepsilon \rightarrow 0$.

Therefore, to sum up, we have proved both $\|I_1\|_{L^2(\Omega)}$ and $\|I_2\|_{L^2(\Omega)}$ go to zero as $\varepsilon \rightarrow 0$. The proposition is proved. \square

5. CONVERGENCE OF THE FORCE-BASED HYBRID METHOD

With the consistency and stability results prepared in the last three sections, we are now ready to prove the main result Theorem 1. The proof follows the spirit of Strang's convergence proof of nonlinear finite difference schemes [37].

As a direct consequence of Corollary 2.3, we have the following

Corollary 5.1 (Higher order expansion). *Under the same assumptions of Theorem 1, there exist positive constants δ and M , so that for any $p > d$ and $f \in W^{15,p}(\Omega) \cap W_{\sharp}^{1,p}(\Omega)$ with $\|f\|_{W^{15,p}} \leq \delta$, denote $\tilde{y} = x + u(x)$ with u the solution of the Cauchy-Born elasticity problem (1.8), we then have*

$$\|\mathcal{F}_{\text{hy}}[\tilde{y}] - f\|_{L^\infty} \leq M\varepsilon^2.$$

Remark. Using the remark under Lemma 2.1, the regularity assumption of f can be relaxed to $W^{5,p}(\Omega)$ with $p > d$.

Proof of Theorem 1. We take \tilde{y} be that given by Corollary 5.1. It is easy to see

$$\int_0^1 \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (y - \tilde{y}) = \mathcal{F}_{\text{hy}}[y] - \mathcal{F}_{\text{hy}}[\tilde{y}].$$

Hence y is the solution of (1.9) if and only if

$$\int_0^1 \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (y - \tilde{y}) = f - \mathcal{F}_{\text{hy}}[\tilde{y}].$$

For any $\kappa \in (3/2, 2)$, we define

$$B = \{y \in X_\varepsilon \mid \|y - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa\}.$$

We define a map $T : B \rightarrow B$ as follows: for any $y \in B$, let $T(y)$ be the solution of the linear system

$$(5.1) \quad \int_0^1 \mathcal{H}_{\text{hy}}[ty + (1-t)\tilde{y}](x) dt \cdot (T(y) - \tilde{y}) = f - \mathcal{F}_{\text{hy}}[\tilde{y}].$$

We first show that T is well defined. Since

$$\|ty + (1-t)\tilde{y} - \tilde{y}\|_{\varepsilon,2} \leq t\|y - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa,$$

which gives that for sufficiently small ε and $d \leq 3$, there holds

$$\|ty + (1-t)\tilde{y} - \tilde{y}\|_{W_\varepsilon^{2,\infty}} \leq \varepsilon^{\kappa-d/2} < \delta,$$

where the constant δ appears in Theorem 5. It follows from Theorem 5 that the problem (5.1) is solvable and

$$(5.2) \quad \begin{aligned} \|T(y) - \tilde{y}\|_{\varepsilon,2} &\leq C\|f - \mathcal{F}_{\text{hy}}[\tilde{y}]\|_{\varepsilon,0} \\ &\leq C\|f - \mathcal{F}_{\text{at}}[\tilde{y}]\|_{\varepsilon,0} + C\|\mathcal{F}_{\text{at}}[\tilde{y}] - \mathcal{F}_{\text{hy}}[\tilde{y}]\|_{\varepsilon,0} \\ &\leq C\varepsilon^2, \end{aligned}$$

where we have used Corollary 5.1. For sufficiently small ε , we have

$$\|T(y) - \tilde{y}\|_{\varepsilon,2} \leq \varepsilon^\kappa.$$

Therefore, $T(y) \in B$ and T is well-defined, which in turn implies $T(B) \subset B$ for sufficiently small ε . Now the existence of y follows from the Brouwer fixed point

theorem. The solution y is locally unique since the Hessian at y is nondegenerate. Let us denote the solution as y_{hy} , we then have from (5.2) that

$$(5.3) \quad \|\tilde{y} - y_{\text{hy}}\|_{\varepsilon,2} \leq C\varepsilon^2.$$

Proceeding along the same line that leads to (5.2) and using Lemma 2.1, we get

$$(5.4) \quad \|\tilde{y} - y_{\text{at}}\|_{\varepsilon,2} \leq C\varepsilon^2.$$

Finally, we conclude that y_{hy} satisfies (1.10) by combining (5.3) and (5.4). \square

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